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# ADAPTIVE FINITE ELEMENT METHOD II: ERROR ESTIMATION



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An adaptive finite element method is developed to solve initial boundary value problems for vector systems of parabolic partial differential equations in one space dimension and time. The differential equations are discretized in space using piecewise linear finite element approximations. Superconvergence properties and quadratic polynomials are used to derive a computationally inexpensive approximation to the spatial component of the error. This technique is coupled with time integration schemes of successively higher orders to obtain an approximation of the temporal and total discretization errors. Computational results indicate that these approximations converge to the exact discretization errors as the mesh is refined.

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## INTRODUCTION

This is the second in a series of four reports whose overall purpose is to describe an adaptive finite element method (AFEM) for solving systems of parabolic partial differential equations. In particular, AFEM attempts to find a numerical solution of an $M$-dimensional system of the form

$$\boldsymbol{u}_t(x,t) + \boldsymbol{f}(x,t,\boldsymbol{u},\boldsymbol{u}_x) = [\boldsymbol{D}(x,t,\boldsymbol{u})\boldsymbol{u}_x(x,t)]_x \ , \ a<x<b \ , \ t>0 \ , \tag{1a}$$

subject to the initial conditions

$$\boldsymbol{u}(x,0) = \boldsymbol{u}^0(x) \ , \ a \le x \le b \tag{1b}$$

and linear separated boundary conditions

$$\left.\begin{aligned} \boldsymbol{A}^l(t)\boldsymbol{u}(a,t) + \boldsymbol{B}^l(t)\boldsymbol{u}_x(a,t) &= \boldsymbol{g}^l(t) \\ \boldsymbol{A}^r(t)\boldsymbol{u}(b,t) + \boldsymbol{B}^r(t)\boldsymbol{u}_x(b,t) &= \boldsymbol{g}^r(t) \end{aligned}\right. \ , \ t>0 \ . \tag{1c}$$

The variables $x$ and $t$ represent spatial and temporal coordinates and denote partial differentiation when they are used as subscripts; $\boldsymbol{u}, \boldsymbol{f}, \boldsymbol{u}^0, \boldsymbol{g}^l$, and $\boldsymbol{g}^r$ are $M$-vectors; and $\boldsymbol{D}, \boldsymbol{A}^l, \boldsymbol{B}^l, \boldsymbol{A}^r$, and $\boldsymbol{B}^r$ are $M \times M$ matrices.

The problem is assumed to be well-posed and parabolic; thus, e.g., $\boldsymbol{D}(x,t,\boldsymbol{u})$ is positive definite. The rows of $\boldsymbol{B}^l$ and $\boldsymbol{B}^r$ are restricted to be either entirely zero or a row of the $M \times M$ identity matrix. When the $i^{th}$ row of $\boldsymbol{B}^l$ or $\boldsymbol{B}^r$ is identically zero, then $A^l_{ii}$ or $A^r_{ii}$ cannot be zero, respectively, and the boundary condition is a Dirichlet (essential) condition. Otherwise, the boundary condition is a Neumann or Robbins (natural) condition. The ultimate goal of AFEM is to determine an approximate solution to Eq. (1) to within a user prescribed error tolerance.

The adaptive strategies utilized by AFEM are (1) error estimation coupled with (2) local mesh refinement (cf., e.g., Adjerid and Flaherty (ref 1), Babuska and Dorr (ref 2), Babuska, Zienkiewicz, Gago, and Oliveira (ref 3), Bank and Weiser (ref 4), Berger and Oliger (ref 5), Bieterman and Babuska (refs 6,7), Moore and Flaherty (ref 8), Shephard (ref 9), Strouboulis and Oden (ref 10), Zienkiewicz and Zhu (ref 11)), and (3) mesh movement (cf., e.g., Adjerid and Flaherty (ref 1), Arney and Flaherty (ref 12), Bell and Shubin (ref 13), Davis and Flaherty (ref 14), Dorfi and Drury (ref 15), Dwyer (ref 16), Ewing, Russell, and Wheeler (ref 17), Hyman (ref 18), Kansa, Morgan, and Morris (ref 19), Miller and Miller (refs 20,21), Petzold (ref 22), Rai and Anderson (ref 23), Russell and Ren (ref 24), Saltzman and Brackbill (ref 25), Smooke and Koszykowski (ref 26), Thompson (ref 27), Verwer, Blom, Furzeland, and Zegeling (ref 28), and White (ref 29)).

The purpose of this report is to describe the error estimating procedures employed by AFEM. Detailed summaries of how AFEM implements its other adaptive strategies are found in separate reports entitled: Adaptive Finite Element Method III: Mesh Refinement (ref 30) and Adaptive Finite Element Method IV: Mesh Movement (ref 31). Furthermore, the report, Adaptive Finite Element Method I: Solution Algorithm and Computational Examples (ref 32), describes how all the adaptive algorithms are implemented in unison and contains results demonstrating the utility of AFEM as a computational tool.

The error estimation performed by AFEM is based on the work of Adjerid and Flaherty (ref 1). Adjerid and Flaherty developed an a posteriori estimate to the spatial discretization error of a finite element method of lines solution for a vector system of parabolic partial differential equations. They discretized the system in space using Galerkin's method with piecewise polynomial finite element approximations of an arbitrary order $p$. The error estimate was calculated using Galerkin's method with piecewise polynomial functions of order $p + 1$. A nodal superconvergence property of the finite element method was used to neglect errors at nodes, and thus, improve computational efficiency. Ordinary differential equations (ODEs) for the finite element solution and error estimation were then integrated in time using the backward difference code DASSL (cf., Petzold (ref 33)).

Adjerid and Flaherty (ref 1) assumed that the temporal discretization error associated with DASSL was negligible compared to the spatial error. Thus, their estimate of the spatial discretization error could be regarded as an estimate of the total error. They used their error estimate to control mesh moving and local mesh refinement procedures that simultaneously attempted to equidistribute the error estimate and satisfy a prescribed global error tolerance. Similar mesh refinement strategies have been used by Bieterman and Babuska (refs 6,7).

Our goal is to develop techniques that simultaneously estimate temporal and spatial discretization errors. With such estimates, mesh refinement and/or moving decisions can be made to reduce the largest component of the error with the least amount of work. For example, if the temporal error is the dominant component of the total error, then one need only adjust the time step in order to improve accuracy. In this way, one avoids needlessly increasing the spatial discretization which would increase the computational complexity unnecessarily. Local and global estimates of the discretization error have been successfully used to control refinement algorithms that attempt to solve partial differential equations to prescribed levels of accuracy (cf., e.g., Babuska, Zienkiewicz, Gago, and Oliveira (ref 3) and Flaherty, Paslow, Shephard, and Vasilakis (ref 34) for a sampling).

As in Adjerid and Flaherty (ref 1), Eq. (1a) is discretized in space using Galerkin's method with piecewise linear finite elements. Temporal discretization, however, is performed by the backward Euler method as opposed to using an ODE code (cf., Coyle and Flaherty (ref 32)). A second solution is calculated using trapezoidal rule integration in time and the difference between the two solutions is used to furnish an estimate of the temporal discretization error. A third solution is obtained using quadratic finite elements and the trapezoidal rule in time. This solution is higher order in space and time than the original piecewise linear finite element-backward Euler solution. Hence, it can be used to provide an estimate of the total discretization error of the piecewise linear finite-element backward Euler solution. Furthermore, the difference between the piecewise linear and quadratic solutions calculated by the trapezoidal rule furnishes an estimate of the spatial discretization error (cf., Moore and Flaherty (ref 8) or Coyle and Flaherty (ref 35)).

At first sight, the above procedure seems expensive; however, nodal superconvergence significantly reduces computational complexity. In the present context, superconvergence implies that finite element solutions converge at a faster rate at mesh point locations than elsewhere in the problem domain (cf., Adjerid and Flaherty (ref 1)). Hence, the error at the nodes may be neglected relative to the error in the interior of the elements when $N$, the number of mesh points, is sufficiently large. Nodal superconvergence has been used by several investigators as a means of constructing a posteriori error estimates in finite element approximations (cf., Adjerid and Flaherty (ref 1), Bieterman and Babuska (refs 6,7), and Coyle and Flaherty (ref 12)). Defect correction methods can also be used to reduce costs associated with the temporal integration (cf., Dahlquist, Björk, and Anderson (ref 36)).

The piecewise linear and quadratic finite element procedures and the temporal integration schemes are outlined in the Numerical Discretization section (cf., Coyle and Flaherty (ref 32) for a more complete description). Derivations of the various error estimates (total, spatial, and temporal) are presented in the Error Decomposition and Estimates section. Then in Convergence Examples, examples that indicate the convergence of the error estimates to the true error and its components are described. Finally, in the last section, a summary of this report is presented.

## NUMERICAL DISCRETIZATION

A weak form of the problem is constructed by multiplying Eq. (1a) by a test function $v(x,t) \in H_0^1$, integrating the result with respect to $x$ from $a$ to $b$, and integrating the diffusive term by parts to obtain

$$(\boldsymbol{v},\boldsymbol{u}_t) + (\boldsymbol{v},\boldsymbol{f}) + A(\boldsymbol{v},\boldsymbol{u}) = \boldsymbol{v}^T \boldsymbol{D} \boldsymbol{u}_x \big|_a^b , \; t>0 , \; \textit{for all } \boldsymbol{v} \in H_0^1 . \tag{2a}$$

The inner product $(v,u)$ and strain energy $A(v,u)$ are defined as

$$(\boldsymbol{v},\boldsymbol{u}) = \int_a^b \boldsymbol{v}^T \boldsymbol{u} \, dx , \; A(\boldsymbol{v},\boldsymbol{u}) = \int_a^b \boldsymbol{v}_x^T \boldsymbol{D} \boldsymbol{u}_x \, dx . \tag{2b,c}$$

Functions $v$ belonging to $H^1$ are required to have finite values of $(v,v)$ and $(v_x,v_x)$. Functions in $H_0^1$ are in $H^1$ and vanish at $x = a$ and/or $b$ if an essential boundary condition is applied there.

Any weak solution $u \in H_E^1$ of Eq. (2a) must also satisfy any essential boundary conditions at $x = a$

$$u_i(a,t) = \left[ g_i^l(t) - \sum_{\substack{j \neq i \\ j=1}}^{M} A_{ij}^l(t) u_j(a,t) \right] \div A_{ii}^l(t) \tag{2d}$$

or at $x = b$

$$u_i(b,t) = \left[ g_i^r(t) - \sum_{\substack{j \neq i \\ j=1}}^{M} A_{ij}^r(t) u_j(b,t) \right] \div A_{ii}^r(t) \tag{2e}$$

when the $i^{th}$ row of $B^l$ and/or $B^r$ is zero, respectively. Natural boundary conditions replace the $i^{th}$ component of $u_x$ at $x = a$ or $b$ in Eq. (2a) when prescribed.

Initial conditions for Eq. (2a) are obtained by $L^2$ projection, i.e.,

$$(v,u) = (v,u^0) \ , \ t = 0 \ , \ for\ all\ v \in H_0^1 \ . \tag{2f}$$

A discrete version of the weak system Eq. (2) is constructed by using finite element-Galerkin procedures in space and finite difference techniques in time on a fully adaptive mesh (one that is both refined and moved as time progresses).

## Spatial Discretization

To discretize Eq. (2a) in space, introduce a time-dependent partition

$$\Pi_N(t) = \{ \ a = x_0 < x_1(t) < x_2(t) < \ldots < x_N = b \ \} \tag{3}$$

of $(a,b)$ into $N$ subintervals $(x_{i-1}(t), x_i(t))$, $i=1,2,\ldots,N$ and approximate $u$ and $v$ by piecewise polynomial functions $U$ and $V$, respectively, with respect to this partition. Thus, the spatially-discrete form of Eq. (2a) consists of finding $U \in S_E^N \subset H_E^1$ such that

$$(V,U_t) + (V,f) + A(V,U) = V^T D U_x\Big|_a^b \ , \ t>0 \ ,$$
$$\textit{for all } V \in S_0^N \subset H_0^1 \ , \tag{4a}$$

$$(V,U) = (V,u^0) \ , \ t=0 \ , \textit{ for all } V \in S_0^N \subset H_0^1 \ . \tag{4b}$$

The spaces $S_E^N$ and $S_0^N$ will consist of either piecewise linear or piecewise quadratic polynomial functions. The spaces of piecewise linear polynomials are denoted $S_E^{N,1}$ and $S_0^{N,1}$ and a basis is easily constructed in terms of the familiar "hat" functions

$$\phi_i(x,t) = \begin{cases} \dfrac{x - x_{i-1}(t)}{x_i(t) - x_{i-1}(t)} \ , & x_{i-1}(t) \le x \le x_i(t) \\ \dfrac{x_{i+1}(t) - x}{x_{i+1}(t) - x_i(t)} \ , & x_i(t) \le x \le x_{i+1}(t) \ . \\ 0 & , \textit{ otherwise} \end{cases} \tag{5}$$

The piecewise linear finite element solution $U_1 \in S_E^{N,1}$ is written in the form

$$U_1(x,t) = \sum_{i=0}^{N} c_i(t)\phi_i(x,t) \tag{6}$$

and determined by solving the ordinary differential system

$$(V_1,U_{1_t}) + (V_1,f(\cdot,t,U_1,U_{1_x})) + A(V_1,U_1) = V_1^T D U_{1_x}\Big|_a^b \ ,$$
$$t>0 \ , \textit{ for all } V_1 \in S_0^{N,1} \ , \tag{7a}$$

$$(V_1,U_1) = (V_1,u^0) \ , \ t=0 \ , \textit{ for all } V_1 \in S_0^{N,1} \ , \tag{7b}$$

where the piecewise linear test functions $V_1 \in S_0^{N,1}$ have a form similar to Eq. (6).

Piecewise quadratic approximations $U_2 \in S_0^{N,2}$ are constructed by adding a "hierarchical" correction $E_2(x,t)$ to $U_1$, i.e.,

$$U_2(x,t) = U_1(x,t) + E_2(x,t) , \tag{8a}$$

where

$$E_2(x,t) = \sum_{i=1}^{N} d_{i-½}(t)\, \psi_{i-½}(x,t) . \tag{8b}$$

The basis $\psi_{i-½}(x,t),\ i=1,2,...,N,$ for the quadratic correction has the form

$$\psi_{i-½}(x,t) = \begin{cases} \dfrac{2[x-x_{i-1}(t)][x-x_i(t)]}{[x_i(t)-x_{i-1}(t)]^2} & , x_{i-1}(t) < x < x_i(t) \\ 0 & , \textit{otherwise} \end{cases} . \tag{9}$$

Piecewise quadratic solutions are determined by solving

$$(V_2,U_{2_t}) + (V_2,f(\cdot,t,U_2,U_{2_x})) + A(V_2,U_2) = V_2^T D U_{2_x}\big|_a^b , \quad t>0 , \textit{ for all } V_2 \in S_0^{N,2} , \tag{10a}$$

$$(V_2,U_2) = (V_2,u^0) , t=0 , \textit{ for all } V_2 \in S_0^{N,2} , \tag{10b}$$

where $V_2$ has a form similar to Eq. (8).

## Temporal Discretization

Discretization in time is performed by integrating, for example, Eq. (4a) over the time step from $t^{n-1}$ to $t^n$ to obtain

$$\sum_{i=1}^{N} \int_{t^{n-1}}^{t^n} \int_{x_{i-1}}^{x_i} V^T U_t + V^T f + V_x^T D U_x \, dx \, dt = \int_{t^{n-1}}^{t^n} V^T D U_x \big|_a^b \, dt \, , \qquad \text{(11a)}$$

$$\textit{for all } V \in S_0^N \, ,$$

$$(V,U) = (V,u^0) \, , \; t=0 \, , \textit{ for all } V \in S_0^N \, . \qquad \text{(11b)}$$

The integration in Eq. (11) will be over an irregular region due to the mesh motion with the test function $V$ having an undesirable time dependency.

In order to overcome this difficulty, introduce a linear transformation

$$x = x_{i-1}^{n-1} + \left(x_{i-1}^{n} - x_{i-1}^{n-1}\right)\tau + \tfrac{1}{2}\Delta x_i^{n-1}(1+\xi) + \tfrac{1}{2}(\Delta x_i^{n} - \Delta x_i^{n-1})\tau(1+\xi), \qquad \text{(12a)}$$

$$t = t^{n-1} + \Delta t^n \tau \qquad \text{(12b)}$$

where

$$\Delta x_i^n = x_i^n - x_{i-1}^n \, , \; \Delta t^n = t^n - t^{n-1} \qquad \text{(12c,d)}$$

and

$$x_i^n = x_i(t^n) \, , \; i = 0,1,\ldots,N \, . \qquad \text{(12e)}$$

This transformation maps the rectangle $\{(\xi,\tau)|-1 \le \xi \le 1, 0 \le \tau \le 1\}$ onto the trapezoidal space-time element whose vertices are

$$(x_{i-1}^{n-1}, t^{n-1}) \, , \; (x_i^{n-1}, t^{n-1}) \, , \; (x_{i-1}^n, t^n) \text{ and } (x_i^n, t^n) \, .$$

The basis elements $\phi_{i-1}(x,t)$ and $\phi_i(x,t)$, the only nonzero ones on $\{(x,t)\,|x_{i-1}(t) \le x \le x_i(t) \, , \, t^{n-1} \le t \le t^n\}$, are transformed to functions with no $\tau$ dependency; thus, $\phi_{i-1}(x,t)$ and $\phi_i(x,t)$ become, respectively,

$$\hat{\phi}_{-1}(\xi) = \tfrac{1}{2}(1-\xi) \text{ , and} \tag{13a}$$

$$\hat{\phi}_{1}(\xi) = \tfrac{1}{2}(1+\xi) \text{ , } -1 \le \xi \le 1 \text{ .} \tag{13b}$$

Define

$$F_i = \int_{t^{n-1}}^{t^n} \int_{x_{i-1}}^{x_i} (V^T U_t + V^T f + V_x^T D U_x) \, dx \, dt \tag{14}$$

and write Eq. (11) as

$$\sum_{i=1}^{N} F_i = \int_0^1 V^T D U_x \big|_a^b \, \Delta t^n d\tau \text{ , } for\ all\ V \in S_0^N \text{ ,} \tag{15a}$$

$$(V,U) = (V,u^0) \text{ , } t=0 \text{ , } for\ all\ V \in S_0^N \text{ .} \tag{15b}$$

by performing the change of variables from $t$ to $\tau$ (cf., Eq. (12b)).

Transforming Eq. (14) from the *(x-t)*-plane to the $(\xi,\tau)$-plane (cf., Eq. (12)) yields

$$F_i = \int_0^1 \int_{-1}^1 \left[ V^T (U x_\xi)_\tau - V^T (U \dot{x})_\xi t_\tau + V^T f x_\xi t_\tau + V_\xi^T D U_\xi \frac{t_\tau}{x_\xi} \right] d\xi \, d\tau \tag{16a}$$

where

$$\dot{x} = \frac{x_\tau}{t_\tau} \text{ .} \tag{16b}$$

Equation (16a) can be simplified further by integrating by parts to obtain

$$F_i = G_i(1) - G_i(0) + \Delta t^n \int_0^1 I_i(\tau) \, d\tau \tag{17a}$$

where

$$G_i(\tau) = \int_{-1}^{1} V^T U x_\xi \, d\xi \;, \tag{17b}$$

$$I_i(\tau) = \int_{-1}^{1} [-V^T(U\dot{x})_\xi + V^T f x_\xi + V_\xi^T D U_\xi \frac{1}{x_\xi}] \, d\xi \;. \tag{17c}$$

Substituting Eq. (17a) into Eq. (15a) then yields

$$\sum_{i=1}^{N} \left[G_i(1) - G_i(0) + \Delta t^n \int_0^1 I_i(\tau) d\tau\right] = \Delta t^n \int_0^1 V^T D U_x|_a^b \, d\tau \;, \quad for\ all\ V \in S_0^N \;, \tag{18a}$$

$$(V,U) = (V,u^0) \;,\; t=0 \;,\; for\ all\ V \in S_0^N \;. \tag{18b}$$

All that remains is to approximate the time integrals in Eq. (18) using a quadrature rule. This is done by using a weighted two-step method, which for Eq. (18) has the form

$$\sum_{i=1}^{N} \left[G_i(1) + G_i(0) + \Delta t^n \theta I_i(1) + \Delta t^n (1-\theta) I_i(0)\right] = \Delta t^n \theta V^T D U_x|_a^b|_{\tau=1} + \Delta t^n (1-\theta) V^T D U_x|_a^b|_{\tau=0} \,, for\ all\ V \in S_0^N \,,\ \theta \in [0,1] \,, \tag{19a}$$

$$(V,U) = (V,u^0) \;,\; t=0 \;,\; for\ all\ V \in S_0^N \;. \tag{19b}$$

Only two choices of $\theta$ are utilized: either $\theta = 1$, which yields the backward Euler method, or $\theta = ½$, which yields the trapezoidal rule.

## ERROR DECOMPOSITION AND ESTIMATES

Strang and Fix (ref 37) demonstrate how the total discretization error of a numerical method for solving parabolic partial differential equations, which couples finite elements in space with finite differences in time, can be decomposed into its spatial and temporal components. They do this by defining an intermediate solution, $U$, that satisfies the finite element discretization (cf., Eq. (4a)) but is integrated exactly in time. Continuing to let $u$ denote the exact solution of the Galerkin problem (cf., Eq. (2)), let $U_\theta$ denote the numerical approximation which satisfies both the finite element equations, and the finite difference equations in time (cf., Eq. (19)). Then the total discretization error, $e$, where

$$e = u - U_\theta \tag{20a}$$

can be bounded as follows:

$$\|e\| = \|u - U + U - U_\theta\| \le \|u - U\| + \|U - U_\theta\| . \tag{20b}$$

Strang and Fix (ref 37) show how the first term of the right-hand side of Eq. (20b), $\|u - U\|$, is strictly an error due to the finite element approximation process, and, as such, dependent only on the spatial discretization. Thus, $\|u - U\|$ is the spatial component of the total discretization error. Similarly, they show that $\|U - U_\theta\|$ is dependent on the temporal discretization and hence represents the temporal component of the total discretization error.

Our goal is to estimate the discretization error per time step in solutions of Eq. (19) obtained by using piecewise linear finite element approximations in space and the backward Euler method in time. It seems most appropriate to gage errors in the $H^1$ norm

$$\|e\|_1 = [(e_x,e_x) + (e,e)]^{1/2} ; \tag{21}$$

however, other metrics may also be used. An error estimate that is global in space and local in time may at first seem unusual, but it is commonly used when spatial finite element approximations are combined with temporal finite difference methods (cf., Thomée (ref 38)).

Let the piecewise linear finite element solutions at time $t^n$ obtained by using backward Euler ($\theta$=1 in Eq. (19)) and trapezoidal rule ($\theta$=½ in Eq. (19)) temporal integration be denoted by $U_1^n$ and $U_{1/2}^n$, respectively. Likewise, let $\hat{U}_{1/2}^n$ denote the piecewise quadratic finite element solution of Eq. (19) at $t^n$ found by using the trapezoidal rule integration in time.

It is known (cf., Strang and Fix (ref 37)) that

$$\|u(\cdot,t^n) - U_1^n(\cdot)\|_1 = O((\Delta t^n)^2) + O(N^{-1}) . \tag{22}$$

Since

$$\|u(\cdot,t^n) - \hat{U}_{1/2}^n(\cdot)\|_1 = O((\Delta t^n)^3) + O(N^{-2}) , \tag{23}$$

one should be able to use the difference between $\hat{U}_{1/2}^n$ and $U_1^n$ to estimate the error in $U_1^n$ ; thus,

$$\|u - U_1^n\|_1 \le \|\hat{U}_{½}^n - U_1^n\|_1 + \|u - \hat{U}_{½}^n\|_1$$
$$\le \|\hat{U}_{½}^n - U_1^n\|_1 + O((\Delta t^n)^3) + O(N^{-2}) \ . \tag{24}$$

The main problem in using $\|\hat{U}_{½}^n - U_1^n\|_1$ as an a posteriori estimate of $\|u - U_1^n\|_1$ is the computational effort required to obtain $\hat{U}_{½}^n$. This cost can be reduced considerably by using the superconvergence property of the finite element method for one-dimensional parabolic systems. Nodal superconvergence enables us to approximate $\hat{U}_{½}^n$ as

$$\hat{U}_{½}^n = U_{½}^n + E_{½}^n \tag{25}$$

where $U_{½}^n$ is obtained by solving Eq. (19) using trapezoidal rule integration and $E_{½}^n$ is obtained by solving Eq. (19) by trapezoidal rule integration with $\hat{U}$ replaced by Eq. (8b). Furthermore, it is only necessary to test Eq. (19) against functions $V \in S_0^{N,2}$, where $S_0^{N,2}$ is a space of quadratic polynomials that vanish on $\Pi_N(t)$.

To summarize, the procedure for obtaining the finite element solution $U_1^n$ and its error estimate $U_{½}^n + E_{½}^n - U_1^n$ for the time step $[t^{n-1},t^n]$ consists of:

1. Determining $U_1^n$ as the solution of

$$\sum_{i=1}^{N}\left[G_i(1) - G_i(0) + \Delta t^n I_i(1)\right] = \Delta t^n V^T D^n U_{1_x}^n\Big|_a^b \ , \qquad \textit{for all } V \in S_0^{N,1} \tag{26a}$$

where

$$G_i(1) = \int_{-1}^{1} V^T U_1^n x_\xi^n \, d\xi \ , \ G_i(0) = \int_{-1}^{1} V^T U_1^{n-1} x_\xi^{n-1} \, d\xi \ , \tag{26b,c}$$

$$I_i(1) = \int_{-1}^{1}\left[-V^T(U_1^n \dot{x}^n)_\xi + V^T f^n x_\xi^n + V_\xi^T D^n U_{1_\xi}^n \frac{1}{x_\xi^n}\right] d\xi \ , \tag{26d}$$

and

$$(V,U_1^0) = (V,u^0) \ , \ t=0 \ , \textit{for all } V \in S_0^{N,1} \ . \tag{26e}$$

2. Determining $U^n_{1/2}$ as the solution of

$$\sum_{i=1}^{N}\left[\tilde{G}_i(1) - \tilde{G}_i(0) + \frac{\Delta t^n}{2}\left[\tilde{I}_i(1) + \tilde{I}_i(0)\right]\right] = \frac{\Delta t^n}{2}\left[V^T D^n U^n_{1/2_x} + V^T D^{n-1} U^{n-1}_{1_x}\right]_a^b , \; for \; all \; V \in S_0^{N,1} \tag{27a}$$

where

$$\tilde{G}_i(1) = \int_{-1}^{1} V^T U^n_{1/2} x^n_\xi \, d\xi \;,\; \tilde{G}_i(0) = \int_{-1}^{1} V^T U^{n-1}_1 x^{n-1}_\xi \, d\xi \,, \tag{27b,c}$$

$$\tilde{I}_i(1) = \int_{-1}^{1}\left[-V^T(U^n_{1/2}\dot{x}^n)_\xi + V^T f^n x^n_\xi + V^T_\xi D^n U^n_{1/2_\xi}\frac{1}{x^n_\xi}\right] d\xi \,, \tag{27d}$$

$$\tilde{I}_i(0) = \int_{-1}^{1}\left[-V^T(U^{n-1}_1\dot{x}^{n-1})_\xi + V^T f^{n-1} x^{n-1}_\xi + V^T_\xi D^{n-1} U^{n-1}_{1_\xi}\frac{1}{x^{n-1}_\xi}\right] d\xi \,, \tag{27e}$$

and

$$(V, U^0_1) = (V, u^0) \;,\; t=0 \;,\; for \; all \; V \in S_0^{N,1} \;. \tag{27f}$$

3. Determining $E^n_{1/2}$ as the solution of

$$\sum_{i=1}^{N}\left[\hat{G}_i(1) - \hat{G}_i(0) + \frac{\Delta t^n}{2}\left[\hat{I}_i(1) + \hat{I}_i(0)\right]\right] = 0 \;, \quad for \; all \; \hat{V} \in \hat{S}_0^{N,2} \tag{28a}$$

where

$$\hat{G}_i(1) = \int_{-1}^{1} \hat{V}^T E^n_{1/2} x^n_\xi \, d\xi \;,\; \hat{G}_i(0) = \int_{-1}^{1} \hat{V}^T E^{n-1}_{1/2} x^{n-1}_\xi \, d\xi \,, \tag{28b,c}$$

and

$$\hat{I}_i(1) = \int_{-1}^{1}\left[-\hat{V}^T(E^n_{1/2}\dot{x}^n)_\xi + \hat{V}^T f^n x^n_\xi + \hat{V}^T D^n E^n_{1/2\,\xi}\frac{1}{x^n_\xi}\right]d\xi\ , \tag{28d}$$

$$\hat{I}_i(0) = \int_{-1}^{1}\left[-\hat{V}^T(E^{n-1}_{1/2}\dot{x}^{n-1})_\xi + \hat{V}^T f^{n-1} x^{n-1}_\xi + \hat{V}^T_\xi D^{n-1} E^{n-1}_{1/2\,\xi}\frac{1}{x^{n-1}_\xi}\right]d\xi\ , \tag{28e}$$

$$(V_2, U^0_1 + E^0_{1/2}) = (V_2, u^0)\ ,\ t = 0\ ,\ \mathit{for\ all}\ V_2 \in S^{N,2}_0\ . \tag{28f}$$

Temporal error estimation is local; thus, we use $U^{n-1}_1$ as an initial condition for the trapezoidal rule integrations in Eqs. (27) and (28). Nodal superconvergence and the hierarchical formulation has uncoupled the piecewise linear and quadratic components of $\hat{U}^n_{1/2}$. The spatial error estimate $E^n_{1/2}$ on the subinterval $(x_{i-1}, x_i)$ is furthermore uncoupled from the error on other subintervals and this significantly reduces the computational complexity associated with solving Eq. (28). The solution of Eq. (27), noted in Step 2, is necessary in order to increase the temporal accuracy of the solution because superconvergence only increases the order of accuracy in space. Some computational savings can generally be obtained, especially for nonlinear problems, by calculating $U^n_{1/2}$ as a defect correction to the backward Euler solution $U^n_1$.

As described above,

$$\bar{e}^n := \|U^n_{1/2} + E^n_{1/2} - U^n_1\|_1 \tag{29}$$

furnishes an estimate to the error $\|u - U^n_1\|_1$ of the backward Euler solution. Equation (29) suggests the inequality

$$\bar{e}^n \le \|U^n_{1/2} - U^n_1\|_1 + \|E^n_{1/2}\|_1\ . \tag{30}$$

The term $\|U^n_{1/2} - U^n_1\|_1$ is the difference between two piecewise linear solutions computed with temporal integration schemes of different orders and can be regarded as a measure of the temporal discretization error. In a similar manner, $\|E^n_{1/2}\|_1$ can be regarded as a measure of the spatial discretization error. Indeed, when the finite element system, Eq. (4), is integrated exactly in time, Adjerid and Flaherty (ref 1) proved that $\|E\|_1$ converges to the exact spatial discretization error $\|u - U\|_1$ as $N \to \infty$ for linear parabolic problems.

## CONVERGENCE EXAMPLES

### Example 1

Consider the linear heat conduction problem

$$u_t = \frac{1}{\pi^2} u_{xx} \ , \ 0 < x < 1 \quad , \quad t > 0 \ , \tag{31a}$$

$$u(x,0) = \sin \pi x \ , \ 0 \le x \le 1 \ , \tag{31b}$$

$$u(0,t) = u(1,t) = 0 \ , \ t > 0 \ . \tag{31c,d}$$

The exact solution of this simple problem is

$$u(x,t) = e^{-t} \sin \pi x \ . \tag{32}$$

We solved Eq. (31) on a uniform mesh with $N$ finite elements for one time step $\Delta t$ using the methods described above and several choices of $N$ and $\Delta t$. The effectivity index

$$\Theta := \frac{\bar{e}^{1}}{\| u(\cdot,\Delta t) - U_1^1 \|_1} \tag{33}$$

(cf., Babuska, Miller, and Vogelius (ref 39)), is used as a means of gaging the accuracy of the error estimate $\bar{e}^1$. Ideally, we would like $\Theta$ not to differ appreciably from unity and to approach unity as $N \to \infty$ and $\Delta t \to 0$.

We present a summary of results for a sequence of calculations performed with $N = 2^m$ and $\Delta t = 1.024 \times 2^{-m}$, $m = 1,\dots,10$, in Figure 1. These results strongly suggest that $\Theta \to 1$ as $m \to \infty$.

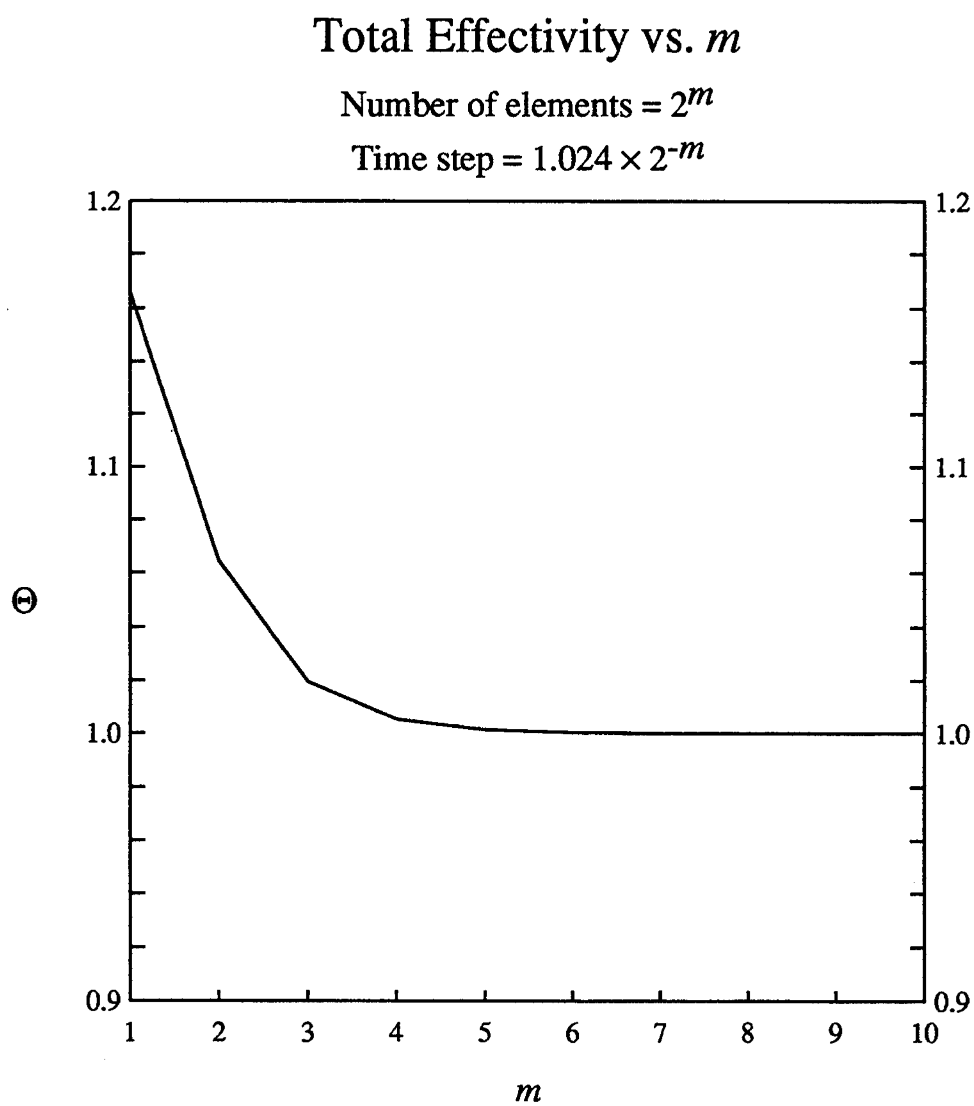


Figure 1. Total effectivity versus discretization for Example 1.

**Example 2**

Consider the linear heat conduction problem

$$u_t + u = \frac{1}{\pi^2} u_{xx} \quad , \quad 0 < x < 1 \quad , \quad t > 0 \; , \tag{34a}$$

$$u(x,0) = 1 \quad , \quad 0 \le x \le 1 \; , \tag{34b}$$

$$u(0,t) = u(1,t) = e^{-t} \quad , \quad t > 0 \; . \tag{34c,d}$$

The exact solution of this simple problem is

$$u(x,t) = e^{-t} \; . \tag{35}$$

We solved Eq. (34) on a uniform mesh with eight finite elements for one time step $\Delta t$ using the methods described above and several choices of $\Delta t$. The temporal effectivity index

$$\Theta_t := \frac{\| U^1_{1/2} - U^1_1 \|_1}{\| u(\cdot,\Delta t) - U^1_1 \|_1} \tag{36}$$

is used as a means of gaging the accuracy of the error estimate $\| U^1_{1/2} - U^1_1 \|_1$. Again, we would like $\Theta_t$ not to differ appreciably from unity and to approach unity as $\Delta t \to 0$, since there is no spatial component to the total discretization error.

We present a summary of results for a sequence of calculations performed with $\Delta t = 1.024 \times 2^{-m}$, $m = 1,...,10$, in Figure 2. These results strongly suggest that $\Theta_t \to 1$ as $m \to \infty$.

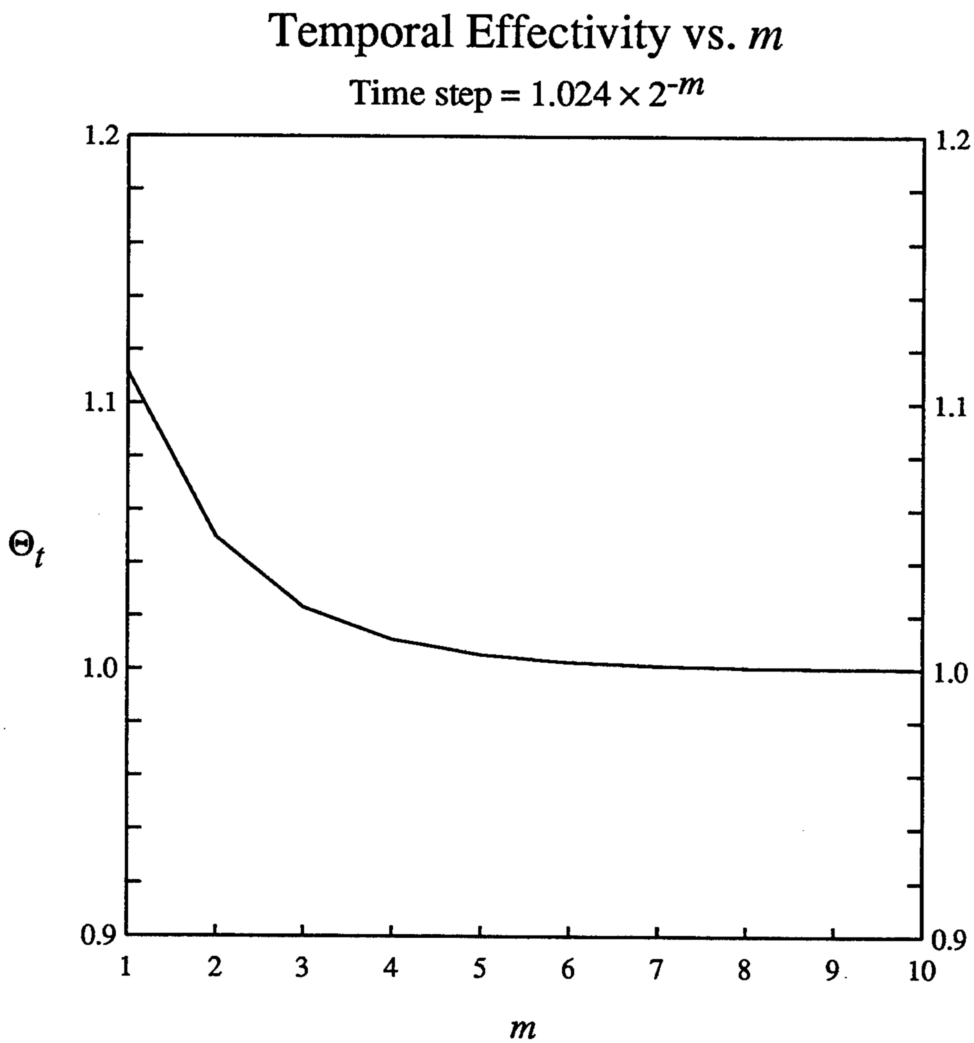


Figure 2. Temporal effectivity versus discretization for Example 2.

## Example 3

Consider the linear heat conduction problem

$$u_t - u = \frac{1}{\pi^2} u_{xx} \quad , \quad 0 < x < 1 \, , \, t > 0 \, , \tag{37a}$$

$$u(x,0) = \sin \pi x \quad , \quad 0 \le x \le 1 \, , \tag{37b}$$

$$u(0,t) = u(1,t) = 0 \quad , \quad t > 0 \, . \tag{37c,d}$$

The exact solution of this simple problem is

$$u(x,t) = \sin \pi x \, . \tag{38}$$

We solved Eq. (37) on a uniform mesh with N finite elements for one time step $\Delta t$ = 0.001 using the methods described above and several choices of $N$. The spatial effectivity index

$$\Theta_s := \frac{\|E^1_{1/2}\|_1}{\|u(\cdot,\Delta t) - U^1_1\|_1} \tag{39}$$

is used as a means of gaging the accuracy of the error estimate $\|E^1_{1/2}\|_1$. Again, $\Theta_s$ should not differ appreciable from unity since for such a small $\Delta t$, there is, effectively, no temporal component to the total discretization error.

We present a summary of results for a sequence of calculations performed with $N = 2^m$, $m = 1,...,10$, in Figure 3.

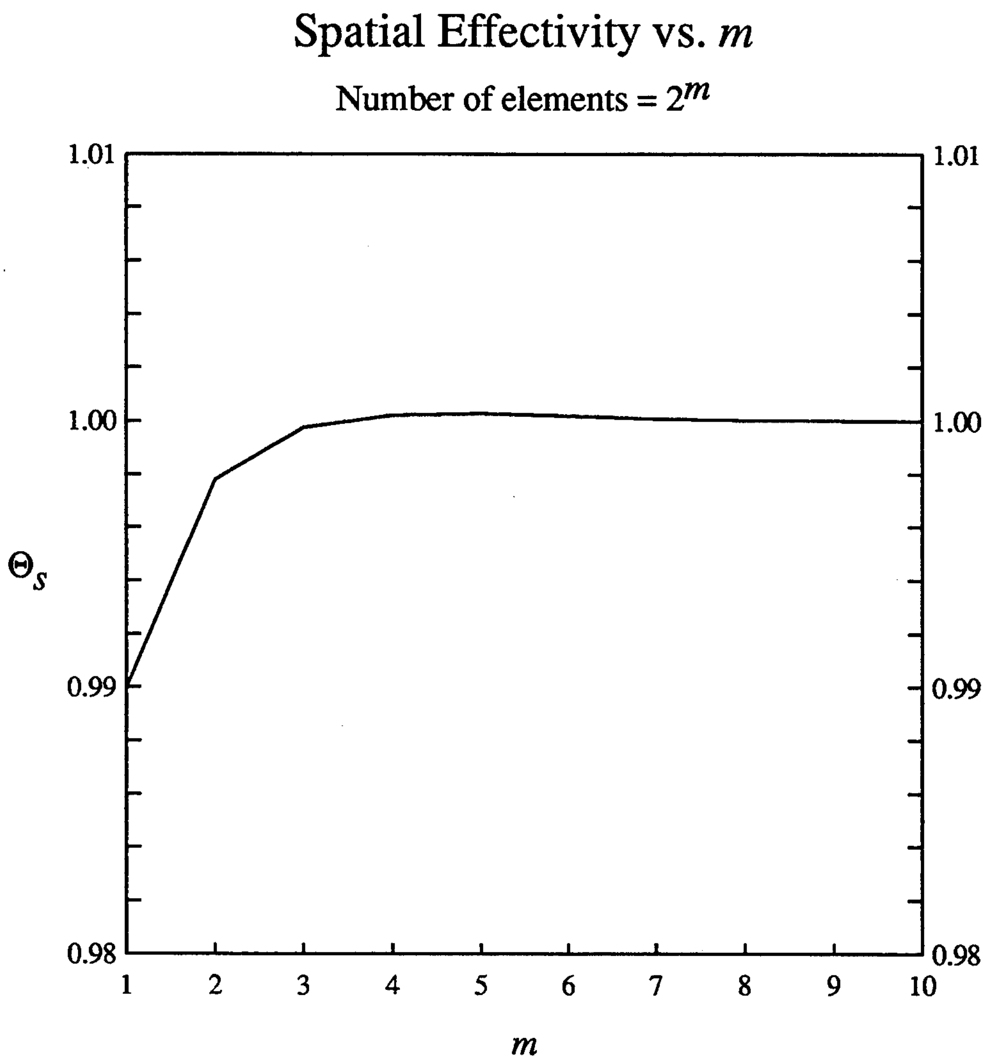


Figure 3. Spatial effectivity versus discretization for Example 3.

## SUMMARY

Methods for calculating a posteriori estimates of the total, spatial, and temporal discretization errors when a vector system of parabolic partial differential equations is solved using piecewise linear finite elements in space and the backward Euler method in time was presented. First, the division of the total discretization error into its spatial and temporal components was shown theoretically. This was followed by a method to approximate these errors numerically. Then it was shown how to obtain these error estimates by using higher-order methods, with nodal superconvergence, in order to improve computational efficiency. Finally, a comparison of the exact and estimated errors was presented in Examples 1, 2, and 3 and in Figures 1, 2, and 3.

Comparison of the exact and estimated errors, presented in Examples 1, 2, and 3, give us some confidence in the accuracy of our error estimates. As indicated by Figures 1, 2, and 3, the three estimates all converge to the true errors as the appropriate discretization levels are increased. Even for coarse levels, results indicate that the estimates do a reasonable job of approximating the exact error (cf., Figures 1, 2, and 3). Thus not only does one get an indication when the total error of the method is too large, but also the dominant component of the error. With this knowledge, one can adjust the appropriate discretization level accordingly. Even in situations when the estimates are not accurate, one gets an indication that refinement is necessary in a particular region.

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